Supplemental Tables and Figures

Evaluation of Computational Docking to Identify PXR Agonists in the ToxCast™ Database

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Supplemental Material

Supplemental Table 1. GoldScores (gs), similarity scores and hybrid scores (hs) of the Sample of compounds from the ToxCast™ database determined in each of the five PXR crystal structures identified by their PDB code.

compound	1m13-gs	hyf-sim	1m13-hs	1nrl-gs	srl-sim	1nrl-hs	1skx-gs	rfp-sim	1skx-hs	2o9i-gs	444-sim	2o9i-hs	2qnv-gs	cdz-sim	2qnv-hs
Mancozeb	37.7	0.1	2.6	42.4	0.1	3.3	39.4	0.1	3.5	37.0	0.2	8.0	34.2	0.0	1.2
Mesosulfuron-methyl	72.1	0.2	15.2	69.8	0.3	23.5	63.1	0.4	26.4	68.7	0.4	29.5	68.7	0.2	16.4
Diethylhexyl phthalate	71.5	0.5	37.5	63.3	0.4	27.2	68.8	0.3	21.9	65.2	0.2	15.1	62.3	0.4	23.2
methylhydrogen phthalate	35.1	0.3	11.4	34.9	0.3	11.9	33.2	0.3	10.3	32.2	0.2	5.0	29.9	0.4	11.1
Bensulide	63.4	0.2	15.6	64.2	0.4	25.3	66.1	0.3	16.7	68.2	0.6	39.1	63.9	0.2	15.7
Foramsulfuron	69.6	0.2	14.3	63.2	0.3	20.1	62.4	0.4	24.1	65.0	0.4	26.7	58.0	0.2	13.4
Bensulfuron methyl	55.7	0.2	11.4	59.1	0.3	19.7	58.3	0.4	24.4	61.0	0.4	26.1	57.5	0.2	13.3
Esfenvalerate	70.5	0.3	21.6	65.5	0.3	21.0	63.4	0.3	20.2	64.9	0.2	11.7	59.5	0.3	20.3
Z,E-Fenpyroximate	71.9	0.3	18.0	61.9	0.4	26.2	62.9	0.5	28.7	67.2	0.3	20.4	56.0	0.3	15.0
Butafenacil	64.7	0.3	20.2	58.6	0.4	25.0	60.4	0.5	28.8	59.7	0.4	21.3	57.9	0.3	18.2
Cypermethrin	66.9	0.4	26.8	60.6	0.4	26.3	63.4	0.4	23.3	65.5	0.2	15.1	57.2	0.4	25.4
Triflusulfuron methyl	69.1	0.2	14.0	62.5	0.4	22.0	60.2	0.4	22.5	60.2	0.5	27.5	53.9	0.2	12.2
Cyfluthrin	66.4	0.4	25.0	59.1	0.4	25.7	62.8	0.4	23.3	60.2	0.2	14.3	58.1	0.4	24.2
Permethrin	63.8	0.4	28.0	56.0	0.5	29.8	56.5	0.3	18.8	58.2	0.3	14.5	57.3	0.5	28.0
Oxasulfuron	63.7	0.2	12.6	58.4	0.3	18.8	61.3	0.4	23.8	60.9	0.4	25.1	55.1	0.2	12.3
Fenarimol	50.9	0.2	11.5	46.1	0.2	11.3	48.7	0.3	13.4	46.3	0.2	9.8	43.5	0.3	10.9
Propiconazole	53.3	0.3	13.7	47.7	0.3	14.4	46.6	0.3	16.3	49.6	0.3	16.2	45.4	0.2	8.6
Fenbuconazole	57.6	0.1	7.5	47.3	0.2	9.5	50.3	0.2	10.2	52.3	0.3	16.7	46.8	0.1	5.0
Prochloraz	60.2	0.3	16.9	52.8	0.3	17.2	52.3	0.4	20.1	52.4	0.3	15.7	51.1	0.2	10.1
Imazalil	47.3	0.2	7.9	45.5	0.3	12.6	45.0	0.3	12.0	46.0	0.2	11.1	42.3	0.2	6.8
Oxadiazon	57.0	0.2	13.7	49.3	0.4	17.6	50.3	0.5	22.6	51.7	0.3	15.2	49.9	0.3	12.8
Alachlor	47.2	0.3	14.1	46.5	0.4	16.5	42.1	0.3	13.9	45.0	0.3	12.9	41.5	0.3	10.8
2,4-D	36.0	0.3	10.3	41.8	0.4	15.9	37.8	0.3	10.7	36.0	0.2	6.6	33.8	0.3	10.8
Diuron	39.5	0.2	6.7	38.7	0.2	8.9	38.9	0.3	10.1	38.7	0.2	7.7	36.3	0.2	6.7
Atrazine	39.7	0.2	6.2	41.8	0.3	10.5	43.3	0.2	10.6	43.0	0.2	9.4	39.4	0.2	7.5
Fipronil	42.5	0.1	4.1	39.7	0.2	7.3	46.6	0.2	10.5	42.3	0.3	14.8	39.1	0.1	4.0
Thiabendazole	42.1	0.1	3.0	40.9	0.1	4.1	40.4	0.2	8.2	40.6	0.1	4.5	35.0	0.1	2.7
Carbaryl	40.0	0.2	8.5	40.8	0.3	11.3	44.4	0.4	17.2	42.4	0.2	8.5	35.1	0.2	8.2

Supplemental Table 2. GoldScores (gs), hybrid scores (hs) for all ToxCast™ compounds docked to the five crystal structures (1m13, 1nrl, 1skx, 2o9i and 2qnv) with 2D similarity Tanimoto scores to the five co-crystal ligands (hyf, srl, rfp, 444 and cdz).

compound	1m13-gs	hyf-sim	1m13-hs	1nrl-gs	srl-sim	1nrl-hs	1skx-gs	rfp-sim	1skx-hs	2o9i-gs	444-sim	2o9i-hs	2qnv-gs	cdz-sim	2qnv-hs
2,2-Bis(4-hydroxyphenyl)-	48.3	0.3	13.2	48.3	0.3	14.2	49.3	0.3	12.5	44.8	0.2	10.0	39.1	0.3	13.4
Acephate	40.1	0.2	8.5	37.8	0.3	12.4	38.1	0.3	11.3	38.5	0.3	12.5	38.0	0.2	8.8
Diethylhexyl phthalate (DI	71.8	0.5	37.6	60.3	0.4	25.9	69.0	0.3	21.9	69.4	0.2	16.1	61.3	0.4	22.8
Diethylhexyl phthalate (DI	71.5	0.5	37.5	63.3	0.4	27.2	68.8	0.3	21.9	65.2	0.2	15.1	62.3	0.4	23.2
Diethyltoluamide	40.7	0.2	8.3	38.0	0.2	9.0	38.9	0.2	8.7	38.9	0.2	8.3	36.7	0.2	7.3
Difenoconazole	62.2	0.2	15.4	55.4	0.3	18.1	55.8	0.4	22.3	57.1	0.3	18.9	50.8	0.2	10.8
Difenzoquat metilsulfate	58.6	0.2	11.7	51.4	0.3	13.9	51.8	0.3	17.0	47.5	0.4	17.6	45.2	0.2	8.9
Dimethenamid	48.0	0.2	11.1	49.2	0.2	11.2	44.2	0.4	16.5	45.0	0.3	11.8	36.9	0.2	7.8
Dimethoate	47.6	0.2	10.5	48.8	0.1	7.2	48.9	0.3	13.9	48.3	0.3	16.8	44.0	0.2	9.6
Dimethomorph	58.3	0.3	18.3	53.8	0.2	12.6	52.2	0.5	24.7	57.4	0.3	19.8	51.0	0.3	14.2
Dimethyl phthalate	36.5	0.3	11.6	36.3	0.2	7.6	35.2	0.3	10.7	34.4	0.2	5.3	31.6	0.4	11.4
Diniconazole-M	53.0	0.3	13.5	44.0	0.2	9.8	49.4	0.4	17.5	49.3	0.3	15.4	44.5	0.3	12.2
Acetamiprid	40.7	0.1	5.8	41.8	0.3	12.6	42.0	0.2	8.5	40.6	0.2	7.2	39.1	0.1	5.3

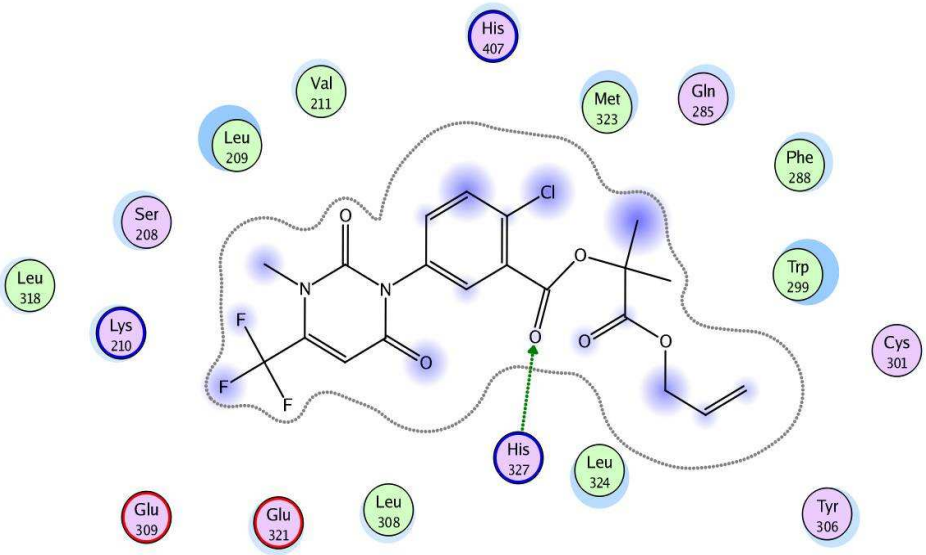
Diphenylamine	39.4	0.1	3.6	37.3	0.2	8.8	37.9	0.2	6.9	36.1	0.1	4.7	34.9	0.1	3.6
Diquat dibromide	42.2	0.1	4.2	40.8	0.3	11.9	35.4	0.2	7.2	40.0	0.2	9.0	32.9	0.1	2.3
Disulfoton	59.3	0.3	17.8	54.8	0.3	17.1	60.3	0.2	9.5	57.7	0.3	18.7	52.5	0.2	11.8
Dithiopyr	55.4	0.3	16.7	49.2	0.3	15.7	52.2	0.3	16.4	52.5	0.3	14.1	48.4	0.3	14.8
Diuron	39.5	0.2	6.7	38.7	0.4	14.8	38.9	0.3	10.1	38.7	0.2	7.7	36.3	0.2	6.7
S-Bioallethrin	60.0	0.7	39.5	51.1	0.3	17.3	56.1	0.4	21.3	50.4	0.2	11.0	54.6	0.7	35.9
Emamectin benzoate	76.7	0.5	36.6	-227.3	0.2	-51.4	52.8	0.7	34.5	-341.0	0.3	-107.4	57.3	0.5	26.8
Endosulfan	38.7	0.3	10.1	43.9	0.5	23.1	40.6	0.2	9.5	38.6	0.4	16.6	34.1	0.3	8.9
EPTC	43.1	0.3	10.8	41.6	0.2	9.1	41.4	0.2	7.2	40.0	0.3	12.1	36.3	0.1	4.8
EPTC	42.9	0.3	10.7	40.1	0.4	17.8	40.9	0.2	7.1	40.3	0.3	12.2	35.4	0.1	4.7
Acetochlor	47.3	0.3	15.2	44.8	0.2	8.8	44.1	0.3	14.5	45.8	0.3	13.1	40.9	0.3	11.5
Esfenvalerate	70.5	0.3	21.6	65.5	0.4	26.2	63.4	0.3	20.2	64.9	0.2	11.7	59.5	0.3	20.3
Ethalfluralin	48.3	0.3	15.4	49.3	0.4	17.7	44.7	0.3	13.2	44.2	0.4	16.2	41.5	0.3	11.8
Ethametsulfuron methyl	65.3	0.2	14.1	55.8	0.3	16.5	59.7	0.4	23.7	57.6	0.4	24.3	52.7	0.2	12.9
Ethephon	27.4	0.2	4.8	33.7	0.3	11.4	32.3	0.1	3.9	29.1	0.3	7.8	28.4	0.2	5.6
Ethofumesate	50.1	0.3	15.9	46.7	0.3	13.8	45.1	0.4	16.1	46.0	0.4	16.1	42.8	0.3	12.9
Ethoprop	53.7	0.3	15.7	51.7	0.3	15.7	49.5	0.1	7.4	51.4	0.3	16.3	44.5	0.2	9.5
Ethylenethiourea	23.8	0.1	1.9	25.9	0.5	11.7	26.3	0.2	5.6	24.1	0.3	6.1	25.1	0.1	2.2
Etoxazole	54.8	0.3	14.7	50.2	0.1	3.9	53.9	0.4	23.7	52.8	0.3	15.5	50.1	0.3	13.5
Etridiazole		0.1	0.0		0.5	0.0		0.3	0.0		0.3	0.0		0.1	0.0
Famoxadone	63.3	0.3	15.8	56.2	0.4	24.6	59.8	0.5	31.5	58.1	0.3	17.8	62.4	0.3	16.8
Acibenzolar-S-Methyl	40.2	0.1	4.5	39.1	0.3	12.2	39.5	0.2	9.6	37.9	0.2	7.6	35.4	0.1	4.3
Fenamidone	55.7	0.2	9.5	51.2	0.4	21.7	52.8	0.4	19.3	51.3	0.3	14.3	49.6	0.2	9.1
Fenamiphos	60.7	0.3	18.9	54.8	0.3	18.5	60.3	0.3	20.4	53.3	0.4	19.5	51.8	0.3	16.4
Fenarimol	50.9	0.2	11.5	46.1	0.3	16.0	48.7	0.3	13.4	46.3	0.2	9.8	43.5	0.3	10.9
Fenbuconazole	57.6	0.1	7.5	47.3	0.3	16.0	50.3	0.2	10.2	52.3	0.3	16.7	46.8	0.1	5.0
Fenhexamid	51.2	0.4	22.3	44.7	0.6	25.8	46.5	0.5	24.3	47.6	0.3	15.8	45.6	0.4	16.9
Fenitrothion	50.4	0.2	11.4	50.1	0.3	16.1	46.5	0.3	13.9	46.0	0.3	15.7	46.4	0.2	11.4
Fenoxaprop-ethyl	63.5	0.3	16.9	53.3	0.4	19.8	54.5	0.5	25.3	55.4	0.2	13.5	49.1	0.2	12.1
Fenoxaprop-ethyl	58.1	0.3	15.5	51.7	0.3	16.9	54.1	0.5	25.1	56.1	0.2	13.7	50.3	0.2	12.4
Fenoxycarb	55.2	0.3	17.1	56.5	0.3	18.6	54.2	0.4	20.3	58.3	0.3	18.1	49.5	0.3	14.4
Fenpropathrin	69.9	0.4	27.3	58.0	0.4	21.1	56.0	0.4	20.1	62.0	0.2	11.2	55.9	0.4	24.5
Acifluorfen	48.0	0.2	11.5	48.9	0.3	12.7	50.1	0.3	17.1	46.8	0.4	16.4	41.1	0.3	10.6
(Z,E)-Fenpyroximate	71.9	0.3	18.0	61.9	0.4	22.2	62.9	0.5	28.7	67.2	0.3	20.4	56.0	0.3	15.0
Fenthion	55.9	0.3	15.6	52.8	0.3	14.6	55.6	0.3	15.5	51.1	0.3	15.5	50.4	0.3	15.4
Fentin	44.2	0.2	6.9	43.8	0.3	14.3	41.2	0.1	5.6	46.5	0.2	7.4	41.3	0.2	7.2
Fipronil	42.5	0.1	4.1	39.7	0.2	8.3	46.6	0.2	10.5	42.3	0.3	14.8	39.1	0.1	4.0
Fluazifop-P-butyl	61.4	0.4	22.9	55.6	0.4	20.1	52.8	0.4	23.5	57.2	0.3	16.7	52.8	0.3	15.2
Fluazifop-P-butyl	64.3	0.4	24.0	52.6	0.2	9.6	53.7	0.4	23.8	55.6	0.3	16.2	51.3	0.3	14.8
Fluazinam	46.1	0.1	6.8	46.5	0.3	12.5	45.3	0.3	11.5	45.8	0.3	14.0	43.5	0.2	6.8
Fludioxonil	40.0	0.2	7.2	39.0	0.2	9.3	44.5	0.4	15.9	40.8	0.2	7.8	35.3	0.2	6.9
Flufenacet	55.1	0.2	11.2	48.2	0.3	14.9	47.3	0.4	17.6	48.7	0.3	16.2	43.0	0.2	8.6
Flufenpyr-ethyl	57.2	0.3	17.8	51.2	0.3	13.3	52.0	0.5	24.8	50.7	0.4	18.8	49.2	0.3	13.8
Alachlor	47.2	0.3	14.1	46.5	0.4	17.7	42.1	0.3	13.9	45.0	0.3	12.9	41.5	0.3	10.8
Flumetralin	52.0	0.2	10.8	48.0	0.3	16.2	47.0	0.2	11.1	49.1	0.4	17.2	46.4	0.2	9.6
Flumetsulam	50.2	0.1	6.5	49.4	0.3	12.9	48.2	0.3	14.3	45.9	0.5	21.6	47.3	0.1	6.5
Flumiclorac-pentyl	63.5	0.4	24.4	58.7	0.4	24.5	58.3	0.6	34.4	59.4	0.3	20.2	51.9	0.3	15.4
Flumioxazin	52.2	0.3	15.4	51.1	0.2	11.4	48.1	0.5	23.8	52.4	0.4	20.2	52.1	0.3	13.7
Fluometuron	38.0	0.2	6.7	36.7	0.2	7.9	37.3	0.3	9.3	39.4	0.2	9.4	36.2	0.2	6.9
Fluoxastrobin	67.0	0.2	12.9	59.6	0.3	18.4	63.4	0.4	25.2	61.7	0.3	17.3	55.6	0.2	10.5
Fluroxypyr	-8.0	0.2	-1.6	38.2	0.3	12.7	37.1	0.4	15.6	29.0	0.2	7.2	31.0	0.2	7.2
Fluroxypyr-meptyl	62.8	0.3	21.9	51.5	0.4	23.0	51.9	0.5	24.3	53.6	0.3	15.1	46.9	0.3	12.1
Flusilazole	51.6	0.1	6.5	47.6	0.3	13.2	46.2	0.2	10.4	48.6	0.3	14.3	43.4	0.1	5.2
Fluthiacet-methyl	58.6	0.2	13.6	54.0	0.4	21.9	52.4	0.4	20.3	53.4	0.4	22.0	54.0	0.2	10.9
Aldicarb	40.0	0.2	6.7	39.3	0.4	16.8	43.0	0.2	10.3	37.8	0.2	9.3	35.4	0.2	6.4
Flutolanil	52.7	0.3	15.3	49.1	0.3	14.5	54.2	0.4	24.2	47.0	0.3	12.2	47.2	0.3	15.1
Folpet	41.3	0.2	8.3	37.9	0.3	11.9	40.5	0.3	14.1	39.6	0.4	14.8	37.9	0.2	8.2
Foramsulfuron	69.6	0.2	14.3	63.2	0.3	21.7	62.4	0.4	24.1	65.0	0.4	26.7	58.0	0.2	13.4
Forchlorfenuron	47.0	0.1	4.5	43.7	0.2	9.7	44.1	0.3	11.5	44.5	0.2	8.2	41.5	0.1	5.1
Formetanate hydrochloric	46.4	0.2	10.1	45.9	0.5	21.5	45.4	0.4	16.0	44.2	0.2	9.1	42.6	0.2	10.1
Fosthiazate	50.0	0.3	16.1	49.6	0.2	9.6	48.0	0.4	17.4	50.0	0.4	20.4	43.2	0.3	12.3
Halosulfuron-methyl	62.1	0.2	10.7	53.7	0.3	17.9	59.3	0.4	24.2	57.4	0.4	22.3	54.7	0.2	10.7
Hexaconazole	50.4	0.3	15.6	47.9	0.2	11.7	46.8	0.3	15.6	44.6	0.4	17.4	42.2	0.2	10.1
Hexazinone	43.4	0.3	12.7	45.0	0.4	18.8	41.0	0.3	13.2	46.0	0.3	13.6	37.9	0.3	9.6
Hexythiazox	51.5	0.2	12.7	50.4	0.5	25.6	46.8	0.4	17.4	51.3	0.4	18.8	51.0	0.2	10.8
Ametryn	49.2	0.2	7.6	45.9	0.3	15.1	48.4	0.2	11.7	44.8	0.2	10.4	43.9	0.2	8.2
Icaridin	44.1	0.3	15.2	43.5	0.3	12.7	40.4	0.3	14.0	40.8	0.4	14.5	38.4	0.3	10.1
Imazalil	47.3	0.2	7.9	45.5	0.3	15.8	45.0	0.3	12.0	46.0	0.2	11.1	42.3	0.2	6.8
Imazamox	52.6	0.3	16.0	48.4	0.3	14.1	50.0	0.5	26.3	54.4	0.2	12.0	48.8	0.3	16.0
Imazapic	50.6	0.3	15.0	46.4	0.1	4.1	42.6	0.5	21.9	45.6	0.2	9.5	44.3	0.3	15.3
Imazapyr	45.6	0.3	13.6	43.0	0.4	17.0	42.0	0.5	21.6	45.6	0.2	9.5	46.0	0.3	15.9
Imazaquin	51.4	0.3	14.6	48.5	0.4	19.0	49.8	0.5	26.7	48.8	0.2	10.5	48.2	0.3	15.8
Imazethapyr	52.8	0.3	17.3	45.9	0.4	18.7	49.2	0.5	24.6	52.3	0.2	11.4	45.2	0.4	16.1
Imidacloprid	43.3	0.2	6.6	42.7	0.3	11.6	44.0	0.2	10.9	42.6	0.4	15.0	40.4	0.1	5.4
Indoxacarb	60.5	0.2	13.7	54.8	0.2	12.8	55.1	0.4	24.3	64.4	0.3	22.2	51.7	0.2	11.0
Iodosulfuron-methyl-sodi	62.5	0.2	12.5	55.4	0.3	19.3	50.6	0.4	18.5	56.1	0.4	23.4	50.8	0.2	10.1
Amitraz	53.8	0.1	7.0	53.8	0.3	16.3	54.6	0.2	11.8	54.8	0.2	8.5	50.1	0.1	7.2
Iprodione	48.8	0.2	11.2	45.0	0.3	12.5	51.3	0.4	20.9	47.4	0.3	13.6	46.2	0.2	11.4
Isazofos	55.9	0.2	11.9	53.4	0.6	33.5	55.0	0.3	18.3	54.0	0.3	18.4	50.7	0.2	10.7
Isoxaben	56.6	0.3	18.6	58.6	0.4	21.5	54.1	0.5	28.9	58.6	0.3	15.5	52.8	0.3	16.5
Isoxaflutole	54.0	0.2	12.1	47.0	0.4	18.4	49.3	0.3	16.0	50.5	0.4	21.3	46.2	0.2	10.3
Lactofen	64.7	0.3	18.5	53.8	0.4	21.5	61.3	0.4	22.1	64.0	0.3	21.6	55.1	0.3	14.8
Lindane	33.6	0.1	3.5	34.6	0.4	15.1	34.1	0.1	2.2	37.3	0.1	3.2	30.2	0.1	3.6
Linuron	41.5	0.2	6.9	40.3	0.3	10.9	40.5	0.3	12.8	39.8	0.3	10.2	36.6	0.2	6.6
Malaoxon	57.9	0.3	17.8	49.7	0.2	11.8	49.9	0.2	9.8	52.4	0.3	16.2	52.3	0.3	13.6
Malathion	59.1	0.3	18.2	54.0	0.4	19.4	55.6	0.2	11.0	55.4	0.3	18.2	56.3	0.3	14.6

Maleic hydrazide	19.5	0.2	3.1	28.1	0.2	5.6	26.4	0.3	8.8	20.4	0.2	4.3	21.8	0.2	4.4
Anilazine	38.0	0.1	3.7	39.1	0.3	10.5	37.2	0.2	9.2	40.1	0.2	8.1	41.2	0.1	4.3
Mancozeb	77.7	0.1	5.3	74.3	0.4	33.0	75.1	0.1	6.7	84.1	0.2	18.2	69.1	0.0	2.5
Maneb	41.8	0.1	2.2	44.9	0.2	9.7	44.0	0.1	4.0	41.2	0.2	8.5	42.2	0.0	1.6
MCPA	37.7	0.3	12.3	42.4	0.4	18.6	39.4	0.3	12.3	37.0	0.2	6.6	34.2	0.3	11.4
Mepiquat chloride	30.5	0.3	7.8	31.7	0.4	11.2	30.1	0.2	5.4	31.5	0.2	7.3	27.8	0.1	4.0
Mesosulfuron-methyl	72.1	0.2	15.2	69.8	0.3	20.5	63.1	0.4	26.4	68.7	0.4	29.5	68.7	0.2	16.4
Mesotrione	51.2	0.3	13.9	51.9	0.0	1.0	47.3	0.3	14.3	51.0	0.4	22.8	47.0	0.3	11.9
Metalaxyl	49.2	0.3	14.2	45.4	0.3	14.9	42.9	0.4	18.7	45.7	0.3	11.9	39.2	0.3	10.5
Methamidophos	33.1	0.1	4.8	36.0	0.2	5.8	35.1	0.2	6.8	29.8	0.3	8.7	30.8	0.2	4.9
Methidathion	53.3	0.2	12.3	50.1	0.4	18.3	49.9	0.4	17.8	49.4	0.3	17.2	47.8	0.2	10.9
2,4-D	36.0	0.3	10.3	41.8	0.3	11.9	37.8	0.3	10.7	36.0	0.2	6.6	33.8	0.3	10.8
Asulam	42.0	0.2	8.2	47.2	0.4	19.5	42.9	0.3	13.4	40.8	0.5	19.0	37.3	0.2	8.5
Methomyl	34.9	0.1	4.0	37.6	0.0	0.0	36.2	0.2	8.3	33.8	0.2	7.4	30.5	0.1	3.8
Methoxychlor	52.9	0.3	15.0	49.0	0.3	13.6	48.8	0.3	13.7	52.0	0.2	11.0	45.7	0.3	14.5
Methoxyfenozide	62.7	0.3	19.9	60.9	0.2	12.2	54.1	0.5	24.7	56.8	0.3	17.0	51.7	0.3	17.8
Methyl cellosolve	20.6	0.2	4.1	23.7	0.2	4.6	24.0	0.2	4.0	21.5	0.1	2.6	19.4	0.2	3.2
Methyl hydrogen phthalat	35.1	0.3	11.4	34.9	0.3	11.2	33.2	0.3	10.3	32.2	0.2	5.0	29.9	0.4	11.1
Metiram-zinc	41.7	0.1	2.2	45.9	0.2	9.0	42.6	0.1	3.9	40.6	0.2	8.4	43.7	0.0	1.6
Metolachlor	51.0	0.3	14.7	47.5	0.1	3.9	46.9	0.4	16.7	53.1	0.3	13.8	40.7	0.2	10.0
Metribuzin	44.6	0.2	8.2	38.2	0.4	15.0	41.8	0.3	12.1	41.6	0.3	11.6	38.0	0.2	7.5
Atrazine	39.7	0.2	6.2	41.8	0.2	6.8	43.3	0.2	10.6	43.0	0.2	9.4	39.4	0.2	7.5
Metsulfuron-methyl	58.1	0.2	11.5	51.8	0.4	19.9	55.0	0.4	22.0	56.9	0.4	23.3	50.2	0.2	11.3
Mevinphos	44.2	0.3	14.4	42.9	0.2	7.4	38.3	0.3	10.4	41.4	0.3	10.8	38.2	0.4	14.0
MGK	48.8	0.4	21.3	46.9	0.3	13.1	48.9	0.4	21.4	47.7	0.3	13.5	47.3	0.3	15.2
Milbemectin	62.3	0.6	36.4	53.5	0.3	18.3	54.0	0.6	31.0	51.5	0.3	15.2	54.6	0.5	30.0
Molinate	38.1	0.2	8.0	37.8	0.3	11.8	36.5	0.2	7.1	38.7	0.3	13.3	36.3	0.1	5.2
Monobutyl phthalate	43.3	0.5	19.6	41.2	0.5	18.5	40.7	0.3	12.7	39.9	0.2	8.2	38.3	0.4	14.0
Monocrotophos	45.7	0.3	12.9	44.0	0.4	15.6	46.5	0.4	17.6	41.0	0.3	12.7	40.6	0.3	12.7
Myclobutanil	49.9	0.2	11.2	45.5	0.3	13.1	46.1	0.2	9.6	48.0	0.3	15.4	44.1	0.1	6.6
Naled	40.2	0.2	7.4	40.9	0.4	14.9	40.0	0.2	6.3	39.8	0.2	9.3	36.6	0.2	7.5
Napropamide	53.1	0.3	15.2	50.4	0.5	22.7	49.2	0.4	19.5	50.5	0.2	12.1	47.7	0.3	12.6
Azamethiphos	51.5	0.2	11.5	47.7	0.3	14.5	49.4	0.5	22.7	47.4	0.3	15.7	47.8	0.2	10.6
Niclosamide-olamine	53.3	0.2	12.5	51.6	0.2	10.1	56.6	0.4	21.6	48.3	0.3	16.6	50.0	0.3	12.5
Nitrapyrin	34.8	0.1	3.6	30.0	0.3	9.2	31.3	0.2	5.3	32.5	0.1	4.5	30.7	0.1	3.6
Norflurazon	47.6	0.2	8.6	43.6	0.3	13.0	42.4	0.4	15.6	43.2	0.3	12.7	41.0	0.2	7.9
Novaluron	57.8	0.2	14.2	52.7	0.3	15.9	52.9	0.4	23.5	53.1	0.3	15.4	50.3	0.3	14.5
Oryzalin	51.4	0.3	13.0	46.7	0.4	20.7	50.4	0.2	12.3	48.0	0.5	24.3	42.6	0.2	7.6
Oxadiazon	57.0	0.2	13.7	49.3	0.5	25.8	50.3	0.5	22.6	51.7	0.3	15.2	49.9	0.3	12.8
Oxamyl	42.8	0.2	7.0	40.6	0.2	6.9	41.3	0.3	11.5	38.5	0.3	9.7	39.4	0.2	7.0
Oxasulfuron	63.7	0.2	12.6	58.4	0.3	19.5	61.3	0.4	23.8	60.9	0.4	25.1	55.1	0.2	12.3
Oxyfluorfen	52.8	0.3	13.2	48.6	0.2	10.4	51.0	0.3	15.4	48.8	0.3	16.7	44.3	0.3	11.1
Oxytetracycline	49.4	0.4	18.5	55.5	0.4	20.5	50.1	0.6	30.5	54.7	0.3	16.3	50.9	0.5	23.2
Azinphos-methyl	54.4	0.2	11.6	51.6	0.4	21.9	56.2	0.4	23.2	51.0	0.4	18.2	53.4	0.2	11.3
Paclobutrazol	53.1	0.3	13.7	46.7	0.3	14.6	54.3	0.3	17.7	48.9	0.3	15.4	45.2	0.3	11.7
Parathion	53.4	0.3	13.8	50.0	0.1	4.0	49.9	0.2	12.3	50.6	0.4	19.6	43.2	0.3	11.2
Parathion-methyl	48.8	0.2	10.5	46.2	0.3	12.3	43.8	0.3	12.0	44.7	0.4	15.7	44.9	0.2	10.5
Pendimethalin	48.9	0.2	11.6	43.8	0.2	8.3	47.9	0.3	12.5	49.0	0.3	13.2	42.6	0.2	10.1
Penoxsulam	55.0	0.2	11.2	52.8	0.2	9.1	52.0	0.4	20.6	54.2	0.5	26.8	51.8	0.2	11.1
Permethrin	63.8	0.4	28.0	56.0	0.4	20.4	56.5	0.3	18.8	58.2	0.3	14.5	57.3	0.5	28.0
Phenoxyethanol	32.8	0.2	8.0	37.4	0.4	15.0	34.0	0.2	7.3	32.0	0.2	5.3	31.4	0.2	7.7
Phosalone	63.0	0.2	14.9	58.4	0.5	26.3	57.2	0.4	24.9	56.3	0.4	20.5	50.0	0.2	11.9
Azoxystrobin	62.6	0.3	19.5	58.3	0.3	19.7	63.4	0.5	32.6	59.5	0.2	12.9	54.4	0.3	18.4
Piperonyl butoxide	63.8	0.4	25.3	59.7	0.3	20.2	54.4	0.4	22.1	60.6	0.2	13.2	52.8	0.3	16.0
Pirimicarb	51.9	0.2	10.8	43.1	0.5	20.3	44.3	0.4	17.9	47.7	0.2	10.2	41.5	0.2	9.4
Pirimiphos-methyl	66.5	0.2	14.4	50.6	0.3	17.0	57.0	0.3	19.7	58.0	0.4	20.5	54.4	0.2	11.6
Prallethrin	60.0	0.7	39.5	50.9	0.3	16.2	51.6	0.4	19.5	49.8	0.2	10.9	47.3	0.7	31.1
Primisulfuron-methyl	67.9	0.2	12.2	54.3	0.4	21.9	56.1	0.4	21.9	57.7	0.4	25.9	53.1	0.2	10.9
Prochloraz	60.2	0.3	16.9	52.8	0.3	17.8	52.3	0.4	20.1	52.4	0.3	15.7	51.1	0.2	10.1
Prodiamine	46.1	0.3	13.6	42.0	0.2	8.0	44.1	0.3	11.7	46.4	0.4	18.3	35.8	0.2	7.4
Profenofos	59.9	0.4	21.0	53.6	0.2	8.3	51.7	0.3	13.7	54.8	0.3	18.7	47.8	0.3	14.8
Prohexadione-calcium	63.0	0.5	31.5	57.1	0.3	16.2	53.7	0.3	15.3	57.6	0.2	11.5	52.7	0.5	25.7
Bendiocarb	40.7	0.3	12.1	41.8	0.5	18.9	46.3	0.6	26.2	41.2	0.2	9.0	36.9	0.3	12.1
Prometon	52.7	0.2	9.2	43.8	0.3	13.6	48.9	0.4	18.9	43.3	0.2	8.1	43.1	0.2	10.0
Prometryn	57.2	0.1	7.4	47.5	0.4	20.1	49.3	0.3	12.7	46.1	0.2	9.1	45.4	0.2	8.3
Propamocarb hydrochlori	47.7	0.3	13.4	41.7	0.3	13.4	41.7	0.3	11.7	43.4	0.3	11.8	40.7	0.2	8.3
Propanil	39.4	0.2	7.4	37.5	0.3	12.1	38.3	0.3	10.1	38.1	0.2	7.0	35.9	0.2	6.6
Propargite	66.3	0.4	25.8	54.5	0.1	7.8	53.6	0.3	14.2	58.9	0.4	25.4	51.7	0.4	18.1
Propazine	50.7	0.1	6.6	41.9	0.3	10.9	46.0	0.3	12.0	44.3	0.2	8.2	41.9	0.2	7.7
Propetamphos	61.4	0.3	18.4	52.4	0.6	29.5	53.2	0.3	15.7	52.7	0.4	20.8	51.7	0.3	14.5
Propiconazole	53.3	0.3	13.7	47.7	0.3	11.9	46.6	0.3	16.3	49.6	0.3	16.2	45.4	0.2	8.6
Propoxur	44.5	0.3	13.1	41.8	0.3	13.5	42.9	0.4	18.7	41.1	0.2	7.9	35.5	0.3	11.6
Propoxycarbazone-sodiun	63.0	0.3	16.1	52.9	0.3	14.4	57.7	0.4	22.4	54.3	0.4	21.5	50.2	0.2	10.0
Benfluralin	44.7	0.3	14.3	46.9	0.1	2.6	40.8	0.3	10.9	48.9	0.4	19.6	40.3	0.2	9.2
Propyzamide	46.2	0.3	12.2	43.0	0.2	9.7	39.9	0.3	12.3	42.4	0.2	8.6	40.8	0.3	12.0
Prosulfuron	63.1	0.2	13.3	53.5	0.4	21.0	55.2	0.4	22.3	56.3	0.5	26.8	55.9	0.2	12.5
Prosulfuron	66.1	0.2	13.9	52.1	0.5	24.3	57.5	0.4	23.2	55.8	0.5	26.6	52.7	0.2	11.8
Prosulfuron	65.2	0.2	13.8	53.9	0.3	18.5	55.3	0.4	22.3	56.4	0.5	26.9	52.3	0.2	11.7
Pymetrozine	41.9	0.1	6.0	40.5	0.3	10.8	42.3	0.3	11.5	40.6	0.3	11.3	39.5	0.1	5.4
Pyraclostrobin	63.5	0.2	11.5	53.6	0.3	18.1	52.0	0.4	22.0	56.7	0.3	16.6	51.0	0.2	9.8
Pyraflufen-ethyl	56.2	0.2	13.9	55.0	0.3	18.8	49.3	0.4	21.4	52.2	0.3	15.6	56.8	0.2	12.1
Pyridaben	63.0	0.2	15.5	55.1	0.4	20.4	52.0	0.3	16.4	55.1	0.3	18.8	55.1	0.3	14.7
Pyrimethanil	46.1	0.1	5.9	41.6	0.5	18.7	43.3	0.3	10.8	42.5	0.2	7.2	39.7	0.1	5.6
Pyriproxyfen	64.2	0.2	15.7	54.9	0.3	15.8	53.4	0.4	19.7	58.2	0.2	11.2	49.1	0.2	12.0
Benomyl	49.6	0.3	13.2	43.5	0.3	14.7	44.8	0.5	21.6	48.1	0.3	13.8	46.6	0.3	11.6
Pyrithiobac-sodium	54.1	0.2	12.0	52.7	0.3	15.3	49.4	0.4	19.1	49.9	0.2	11.9	46.0	0.2	10.2

Quinclorac	39.2	0.2	8.2	37.7	0.3	13.1	38.2	0.3	12.2	37.2	0.2	7.3	33.7	0.2	7.7
Quinoxyfen	48.8	0.2	8.3	47.8	0.3	16.7	46.1	0.3	13.3	48.6	0.2	9.0	42.1	0.2	7.9
Quizalofop-ethyl	62.7	0.3	17.2	58.3	0.4	20.7	52.8	0.4	23.1	56.9	0.2	12.5	52.5	0.3	13.3
Resmethrin	63.0	0.5	29.5	57.0	0.3	19.5	58.8	0.4	21.9	59.6	0.2	12.9	55.1	0.5	28.9
Rimsulfuron	70.2	0.2	14.8	60.6	0.2	12.3	62.7	0.4	24.4	59.3	0.4	24.5	56.4	0.2	12.6
Rotenone	59.4	0.4	23.8	57.0	0.2	10.4	47.1	0.5	24.2	57.5	0.2	11.2	52.6	0.4	20.2
Sethoxydim	59.7	0.5	30.4	51.2	0.3	16.5	53.5	0.4	20.2	53.4	0.4	18.7	47.0	0.4	19.6
Simazine	41.5	0.1	5.2	39.9	0.2	8.4	40.4	0.2	9.5	38.8	0.2	8.1	36.5	0.2	5.7
Bensulfuron-methyl	55.7	0.2	11.4	59.1	0.3	19.0	58.3	0.4	24.4	61.0	0.4	26.1	57.5	0.2	13.3
Spirodiclofen	61.0	0.6	35.2	50.4	0.4	17.7	50.1	0.5	24.0	53.0	0.3	14.4	49.9	0.5	24.0
Spiroxamine	51.9	0.4	21.0	48.2	0.2	11.3	46.6	0.4	17.4	50.7	0.3	15.8	46.5	0.3	13.6
Sulfentrazone	55.7	0.2	9.3	43.8	0.3	11.6	47.4	0.3	16.4	45.1	0.4	18.1	49.2	0.2	8.7
TCMTB	48.4	0.1	4.1	45.0	0.6	27.6	43.8	0.2	7.7	44.0	0.2	8.0	41.0	0.1	3.8
Tebufenozide	59.5	0.3	15.9	55.5	0.1	7.5	52.1	0.3	16.0	59.3	0.3	17.6	50.7	0.3	13.6
Tebufenpyrad	62.5	0.2	13.7	54.6	0.3	17.9	55.4	0.3	19.3	56.2	0.3	15.7	55.1	0.2	11.0
Tebupirimfos	64.5	0.3	18.4	60.3	0.4	25.5	55.3	0.3	15.7	55.6	0.3	18.1	54.1	0.3	15.6
Tebuthiuron	45.5	0.1	6.5	39.8	0.4	14.6	40.4	0.3	11.6	40.5	0.2	10.0	41.2	0.2	6.4
Tefluthrin	57.9	0.4	21.7	44.0	0.1	3.9	48.6	0.3	13.2	51.6	0.2	12.5	47.1	0.4	19.7
Bensulide	63.4	0.2	15.6	64.2	0.2	14.6	66.1	0.3	16.7	68.2	0.6	39.1	63.9	0.2	15.7
Tepraloxydim	57.1	0.4	23.4	49.5	0.4	19.1	52.3	0.3	18.1	53.8	0.4	19.0	49.9	0.4	17.5
Terbacil	38.8	0.3	11.7	38.0	0.2	7.1	35.4	0.4	12.9	36.7	0.3	11.2	34.2	0.3	11.2
Tetraconazole	49.5	0.1	6.3	45.5	0.5	21.8	44.8	0.2	10.8	46.7	0.3	14.6	43.1	0.1	5.9
Tetramethrin	57.1	0.4	25.3	51.0	0.4	21.4	53.1	0.5	26.5	53.6	0.3	17.6	50.4	0.4	20.5
Thiabendazole	42.1	0.1	3.0	40.9	0.1	6.0	40.4	0.2	8.2	40.6	0.1	4.5	35.0	0.1	2.7
Thiacloprid	45.4	0.1	6.3	44.3	0.3	13.1	43.4	0.2	8.4	43.4	0.3	13.2	45.2	0.1	5.2
Thiamethoxam	43.4	0.2	7.3	43.6	0.4	16.8	43.5	0.3	12.3	41.9	0.3	13.2	38.6	0.2	5.8
Thiazopyr	53.6	0.3	14.0	48.3	0.2	9.4	50.5	0.4	18.1	52.4	0.3	16.6	45.0	0.2	10.9
Thidiazuron	41.8	0.1	3.4	41.4	0.3	14.1	42.0	0.3	10.9	41.2	0.3	10.3	38.9	0.1	4.0
Thiobencarb	51.6	0.2	11.0	47.5	0.3	14.6	46.5	0.2	9.2	48.9	0.3	14.2	44.0	0.2	9.3
2,4-DB	38.1	0.3	13.2	48.1	0.3	15.6	41.3	0.3	12.8	39.8	0.2	9.7	38.9	0.3	12.7
Bensulide	62.7	0.2	15.4	64.1	0.3	20.1	68.1	0.3	17.2	69.0	0.6	39.6	60.0	0.2	14.8
Thiodicarb	64.6	0.2	10.6	53.6	0.3	14.0	55.5	0.3	14.5	59.0	0.3	18.9	52.9	0.2	9.4
Thiophanate-methyl	60.8	0.2	13.5	51.6	0.5	23.3	58.8	0.4	24.0	53.2	0.3	13.6	48.3	0.3	12.7
Thiram	49.4	0.1	3.7	47.0	0.3	12.8	44.1	0.1	4.2	45.0	0.2	9.7	45.5	0.1	3.7
Tralkoxydim	58.6	0.4	25.1	50.3	0.2	11.6	51.4	0.4	20.1	53.6	0.3	15.8	48.2	0.4	20.0
Triadimefon	51.7	0.2	11.6	47.2	0.5	25.7	45.6	0.4	18.7	48.4	0.3	13.1	44.0	0.2	10.6
Triadimenol	52.9	0.2	11.9	45.8	0.4	18.7	48.1	0.4	19.7	47.9	0.3	13.7	44.1	0.2	10.7
Tri-allate	55.2	0.2	9.4	48.4	0.2	9.2	46.3	0.2	7.6	45.3	0.3	12.5	42.8	0.2	8.0
Triasulfuron	62.6	0.2	13.9	55.5	0.2	11.1	55.9	0.4	21.5	58.9	0.5	26.8	54.0	0.2	12.7
Tribenuron-methyl	63.6	0.2	12.6	54.9	0.3	19.1	59.4	0.4	22.8	59.4	0.4	25.2	51.8	0.2	10.9
Tribufos	66.0	0.3	18.3	55.0	0.2	10.1	58.9	0.1	8.1	62.0	0.3	19.0	55.7	0.2	10.9
Bensulide	63.6	0.2	15.7	65.6	0.3	17.6	66.8	0.3	16.9	65.3	0.6	37.5	62.4	0.2	15.3
Trichlorfon	38.1	0.2	7.8	38.9	0.4	13.7	35.8	0.2	6.7	34.9	0.3	8.7	37.2	0.2	8.4
Triclopyr	36.3	0.2	7.9	41.3	0.3	11.9	37.8	0.4	14.0	39.7	0.2	8.1	34.9	0.2	8.2
Triclosan	46.4	0.2	11.1	45.5	0.2	9.7	43.9	0.3	11.8	44.3	0.2	7.3	42.1	0.3	11.3
Trifloxystrobin	65.6	0.3	16.9	54.1	0.2	12.0	57.5	0.3	17.9	55.8	0.3	17.9	54.3	0.3	14.1
Trifloxysulfuron-sodium	60.9	0.2	13.0	53.7	0.4	22.8	56.3	0.4	21.6	53.4	0.5	24.1	53.6	0.2	11.3
Triflumizole	51.2	0.2	10.8	47.3	0.4	19.2	49.0	0.3	15.0	47.2	0.3	13.4	45.8	0.1	6.6
Trifluralin	50.0	0.3	15.2	42.0	0.4	16.7	41.9	0.3	10.7	43.8	0.4	17.7	42.3	0.2	9.0
Triflusulfuron-methyl	69.1	0.2	14.0	62.5	0.4	23.9	60.2	0.4	22.5	60.2	0.5	27.5	53.9	0.2	12.2
Triticonazole	55.4	0.4	21.1	48.1	0.4	16.9	49.4	0.4	20.1	43.7	0.4	16.8	45.1	0.3	14.8
Vinclozolin	44.9	0.3	13.4	48.5	0.4	19.0	44.3	0.5	22.4	45.7	0.3	13.7	39.8	0.3	12.8
Bentazone	40.9	0.2	9.2	40.9	0.1	6.1	40.4	0.4	16.1	40.5	0.4	15.8	38.8	0.2	9.3
Zoxamide	57.7	0.4	23.5	44.9	0.3	14.4	49.9	0.4	20.7	47.2	0.3	13.0	44.1	0.3	15.0
Bifenazate	52.6	0.2	12.2	48.2	0.3	15.3	49.8	0.5	22.5	54.6	0.2	12.7	53.2	0.3	14.4
Bifenthrin	58.2	0.4	20.9	56.2	0.6	33.4	56.8	0.3	16.0	56.9	0.3	14.4	52.8	0.4	21.1
Bisphenol A	44.1	0.4	16.5	49.9	0.3	15.9	43.1	0.3	12.0	44.6	0.2	7.5	36.6	0.5	17.2
Boscalid	53.9	0.1	6.0	46.9	0.6	27.3	51.0	0.3	15.8	51.0	0.2	9.3	46.9	0.1	5.7
Bromacil	38.9	0.3	11.4	40.9	0.3	13.6	35.2	0.4	13.1	37.5	0.3	11.7	35.1	0.3	9.6
Bromoxynil	30.5	0.2	6.8	34.8	0.3	12.0	32.2	0.2	7.0	31.3	0.2	4.8	27.6	0.3	6.9
2,5-Pyridinedicarboxylic a	46.9	0.3	16.0	43.8	0.3	13.9	41.9	0.3	14.4	47.7	0.2	10.6	46.5	0.3	12.3
Buprofezin	56.8	0.2	11.4	48.4	0.2	9.4	50.7	0.3	14.6	47.7	0.3	13.3	44.8	0.2	9.6
Butachlor	55.6	0.4	19.8	53.3	0.3	16.4	50.9	0.3	17.2	52.0	0.3	16.2	47.2	0.3	12.8
Butafenacil	64.7	0.3	20.2	58.6	0.2	14.4	60.4	0.5	28.8	59.7	0.4	21.3	57.9	0.3	18.2
Butralin	52.3	0.3	14.9	52.1	0.5	25.0	49.6	0.3	13.3	53.9	0.3	15.7	45.9	0.3	12.2
Butylate	46.0	0.2	9.9	40.5	0.4	15.9	39.3	0.2	6.4	40.7	0.2	9.7	38.1	0.2	6.2
Captan	39.6	0.2	9.4	39.0	0.1	3.9	39.4	0.3	13.0	40.4	0.4	16.7	36.5	0.2	8.7
Carbaryl	40.0	0.2	8.5	40.8	0.5	19.7	44.4	0.4	17.2	42.4	0.2	8.5	35.1	0.2	8.2
Carboxin	45.7	0.3	13.2	44.1	0.4	15.7	43.5	0.5	20.8	42.9	0.3	12.6	41.4	0.3	11.1
Carfentrazone-ethyl	58.7	0.2	13.2	54.7	0.2	8.6	52.6	0.4	19.7	52.1	0.3	16.1	52.6	0.2	11.8
2-Phenylphenol	37.2	0.2	9.1	44.0	0.4	15.7	39.6	0.2	9.2	35.5	0.1	4.4	36.0	0.3	10.0
Chlorethoxyfos	51.7	0.2	11.7	48.2	0.2	10.7	46.0	0.1	5.9	49.9	0.3	17.2	42.3	0.2	9.5
Chloridazon	35.9	0.1	5.1	37.1	0.3	10.1	38.8	0.3	12.4	36.8	0.2	9.1	33.5	0.2	5.2
Chloroneb	36.3	0.3	9.7	35.9	0.3	11.9	35.0	0.3	9.5	35.9	0.1	5.3	33.4	0.3	10.0
Chlorpropham	40.5	0.2	9.1	38.1	0.3	9.7	38.3	0.3	12.0	39.7	0.2	9.1	36.4	0.3	9.1
Chlorpyrifos oxon	53.8	0.3	14.3	53.8	0.3	16.2	48.3	0.4	16.9	48.5	0.3	14.1	42.2	0.3	11.3
Chlorpyrifos-methyl	49.3	0.2	10.3	47.4	0.4	16.6	46.1	0.4	17.0	47.4	0.3	14.6	42.9	0.2	9.7
Chlorsulfuron	56.0	0.2	10.7	50.2	0.3	16.2	51.1	0.4	19.0	49.7	0.4	21.2	48.1	0.2	10.4
Chlorsulfuron	56.5	0.2	10.8	50.5	0.4	22.0	51.5	0.4	19.1	51.7	0.4	22.1	47.6	0.2	10.3
Cinmethylin	53.5	0.5	26.8	44.9	0.2	8.2	50.3	0.4	22.1	50.5	0.2	10.5	46.6	0.4	19.8
3-Iodo-2-propynylbutylca	39.7	0.3	10.1	38.8	0.2	8.2	39.8	0.2	9.7	41.1	0.3	11.0	38.7	0.2	7.2
cis-Captafol	47.0	0.2	11.2	43.6	0.3	12.8	41.4	0.3	13.6	45.8	0.4	18.9	39.2	0.2	9.3
Clodinafop-propargyl	56.7	0.3	16.0	52.5	0.2	12.9	49.6	0.4	21.3	50.7	0.2	12.2	51.8	0.3	14.8
Clofentezine	53.2	0.1	4.4	45.0	0.3	11.4	52.4	0.2	9.0	44.4	0.2	7.8	44.8	0.1	4.0
Clomazone	41.8	0.3	13.1	42.9	0.3	10.9	40.4	0.4	16.2	40.8	0.3	13.4	42.1	0.3	11.8
Cloprop	37.6	0.3	11.1	40.1	0.2	9.5	34.8	0.3	10.1	35.2	0.2	5.8	33.2	0.3	11.0

Clopyralid	30.2	0.2	6.0	34.2	0.2	6.3	33.4	0.3	9.9	28.8	0.2	4.5	24.3	0.2	5.4
Clopyralid-olamine	39.3	0.2	8.6	40.4	0.3	10.3	45.5	0.3	15.0	38.0	0.2	9.0	36.2	0.2	7.8
Clorophene	43.8	0.3	11.9	44.8	0.3	14.6	43.5	0.2	10.2	41.8	0.2	7.7	40.2	0.3	12.4
Clothianidin	43.9	0.1	4.7	43.5	0.4	15.7	38.4	0.2	9.5	41.2	0.3	11.6	38.6	0.1	4.4
Coumaphos	62.0	0.4	22.6	55.8	0.3	17.8	56.7	0.4	20.6	54.7	0.4	19.4	55.0	0.4	20.5
3-Iodo-2-propynylbutylca	39.2	0.3	10.0	39.3	0.4	15.5	38.0	0.2	9.2	41.4	0.3	11.1	38.5	0.2	7.1
Cyanazine	47.7	0.2	8.5	40.9	0.2	6.7	45.7	0.2	11.2	45.8	0.2	10.8	43.5	0.2	9.3
Cyazofamid	52.0	0.2	8.1	46.8	0.3	15.9	47.2	0.3	13.1	47.4	0.4	18.4	44.0	0.2	7.3
Cyclanilide	46.9	0.3	14.8	43.7	0.2	8.5	46.2	0.5	22.4	43.5	0.3	12.9	40.8	0.4	15.2
Cycloate	43.6	0.3	12.6	40.6	0.3	10.1	42.3	0.2	8.5	43.7	0.4	16.4	37.5	0.2	7.2
Cyfluthrin	66.4	0.4	25.0	59.1	0.5	26.6	62.8	0.4	23.3	60.2	0.2	14.3	58.1	0.4	24.2
Cyhalofop-butyl	51.9	0.3	15.6	52.0	0.3	17.3	49.8	0.4	17.6	49.5	0.2	10.5	45.9	0.3	15.3
Cymoxanil	37.6	0.2	7.9	40.6	0.4	14.3	39.6	0.3	11.9	36.2	0.3	9.4	34.5	0.2	7.8
Cypermethrin	66.9	0.4	26.8	60.6	0.1	6.2	63.4	0.4	23.3	65.5	0.2	15.1	57.2	0.4	25.4
Cyproconazole	47.2	0.2	11.3	46.9	0.4	16.9	45.8	0.3	14.0	46.4	0.4	16.9	42.8	0.2	9.5
6-Deisopropylatrazine	30.7	0.1	3.3	37.2	0.3	10.4	34.2	0.2	7.5	30.6	0.2	6.4	29.5	0.1	4.0
Cyprodinil	49.8	0.1	6.1	46.5	0.4	17.2	47.5	0.2	11.5	45.8	0.2	8.3	47.4	0.1	5.4
Cyromazine	33.2	0.1	3.3	35.4	0.4	15.3	37.8	0.2	8.9	30.7	0.2	5.9	30.8	0.1	4.0
Daminozide	33.9	0.3	8.8	34.8	0.4	13.7	35.9	0.3	11.9	32.2	0.3	8.7	34.4	0.3	8.9
Dazomet	34.1	0.2	5.4	34.1	0.3	10.3	33.9	0.2	6.8	33.9	0.3	8.6	31.6	0.1	4.2
d-cis,trans-Allethrin	60.4	0.7	39.8	50.1	0.4	21.7	52.9	0.4	20.1	51.8	0.2	11.3	47.4	0.7	31.2
Diazinon	59.6	0.3	15.1	56.1	0.3	18.4	57.9	0.3	17.7	58.6	0.3	19.3	53.0	0.3	13.5
Diazoxon	57.3	0.3	15.5	51.7	0.4	21.7	54.0	0.3	17.3	54.1	0.3	15.0	50.3	0.3	13.6
Dibutyl phthalate	54.7	0.4	24.2	49.5	0.4	17.6	50.7	0.3	15.6	51.0	0.2	10.4	51.7	0.4	18.4
Dibutyl phthalate	53.3	0.4	23.6	48.4	0.3	16.5	51.6	0.3	15.9	49.9	0.2	10.1	51.1	0.4	18.2
Dicamba	34.2	0.3	11.9	35.8	0.3	9.9	36.4	0.3	12.7	34.8	0.2	6.5	29.0	0.4	11.3
Abamectin	-13.2	0.5	-6.8	27.3	0.3	7.4	57.9	0.6	34.0	-158.0	0.3	-43.8	55.0	0.5	29.6
Dichlobenil	28.5	0.1	3.2	30.2	0.1	4.3	29.0	0.1	3.6	28.8	0.1	2.7	25.5	0.1	3.3
Dichloran	25.8	0.1	2.9	35.7	0.4	13.5	31.3	0.2	5.6	29.7	0.2	6.9	26.8	0.1	3.3
Dichlorprop	37.9	0.3	11.8	40.5	0.3	14.1	36.8	0.3	11.9	36.8	0.2	5.9	34.9	0.4	12.2
Dichlorvos	37.4	0.2	8.4	39.0	0.4	13.7	37.3	0.2	6.9	36.5	0.3	9.7	35.6	0.3	8.9
Diclofop-methyl	51.2	0.3	16.0	50.8	0.2	11.0	48.9	0.4	17.8	50.7	0.2	8.5	45.8	0.3	16.0
Diclofop-methyl	53.8	0.3	16.8	50.0	0.4	17.8	49.5	0.4	18.1	52.7	0.2	8.8	47.0	0.3	16.4
Diclofop-methyl	52.5	0.3	16.4	53.9	0.3	15.3	49.3	0.4	18.0	50.8	0.2	8.5	45.2	0.3	15.8
Diclosulam	53.7	0.2	9.7	51.9	0.5	27.5	51.1	0.3	17.5	53.3	0.5	25.5	49.5	0.2	8.8
Dicofol	48.9	0.3	12.5	41.2	0.1	3.4	43.7	0.2	8.1	43.4	0.2	10.0	41.9	0.3	12.1
Dicrotophos	47.7	0.3	13.9	41.3	0.5	18.7	40.9	0.3	14.0	41.2	0.3	12.9	42.8	0.3	13.7

Supplemental Figure 1. Compounds mapped to 1m13 (Chrencik et al. 2005). A. Butafenacil, B. β–Cyfluthrin, C. Mancozeb and D. Permethrin. Schematic representations of the ligands in the binding site were generated using LIGX option in MOE (Chemical Computing Group, Montreal, Canada). The binding site residues are colored by their nature, with hydrophobic residues in green, polar residues in purple and charged residues highlighted with bold contours.



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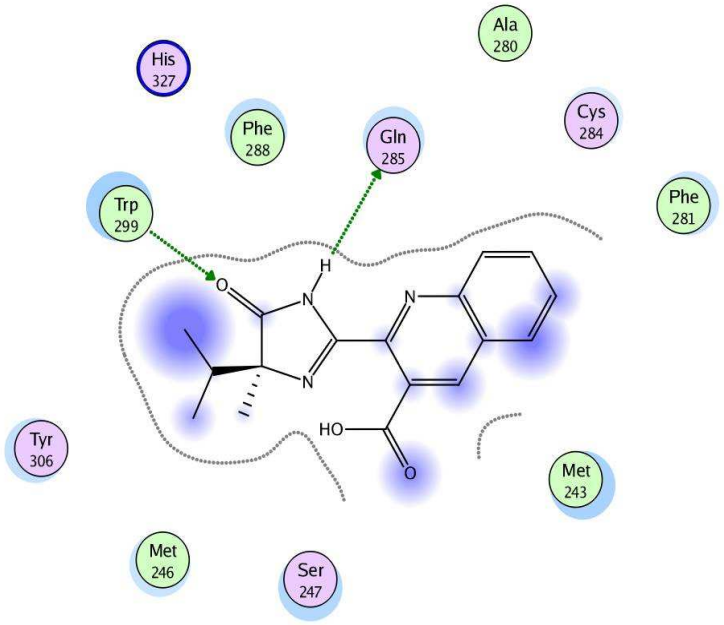
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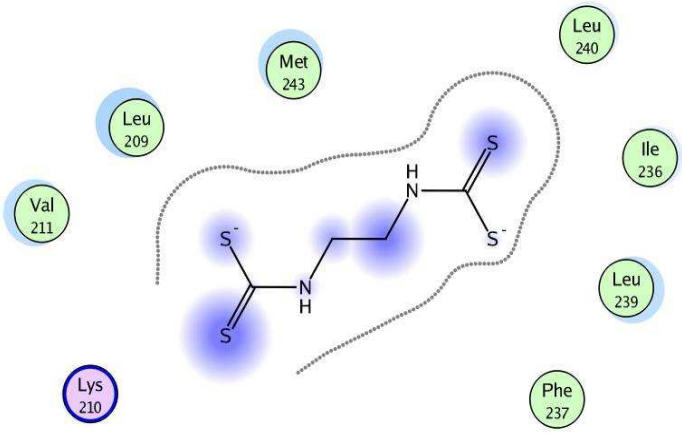
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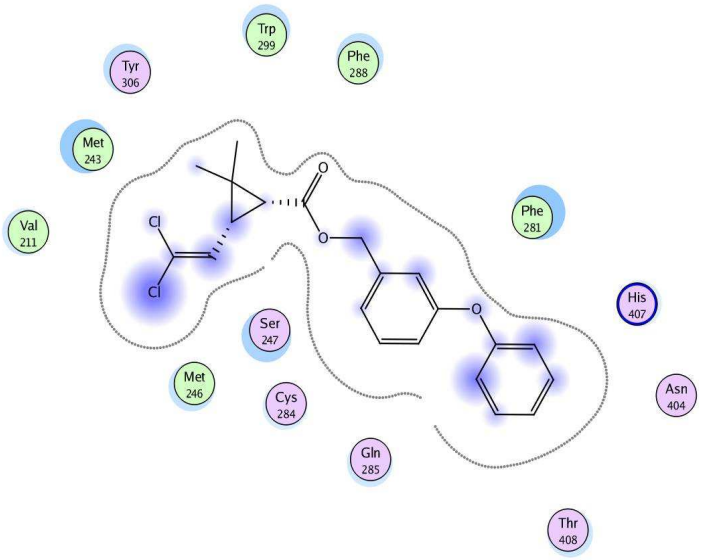
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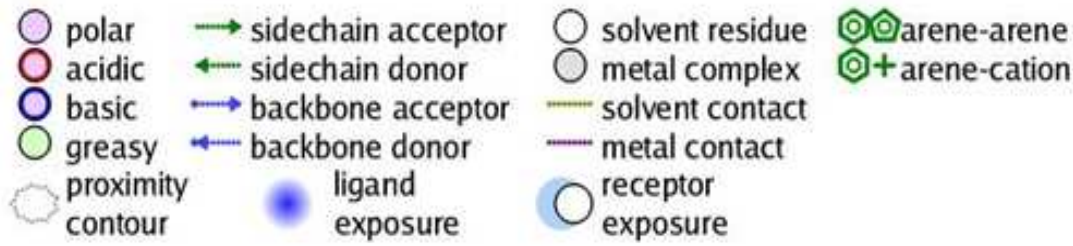
D

Legend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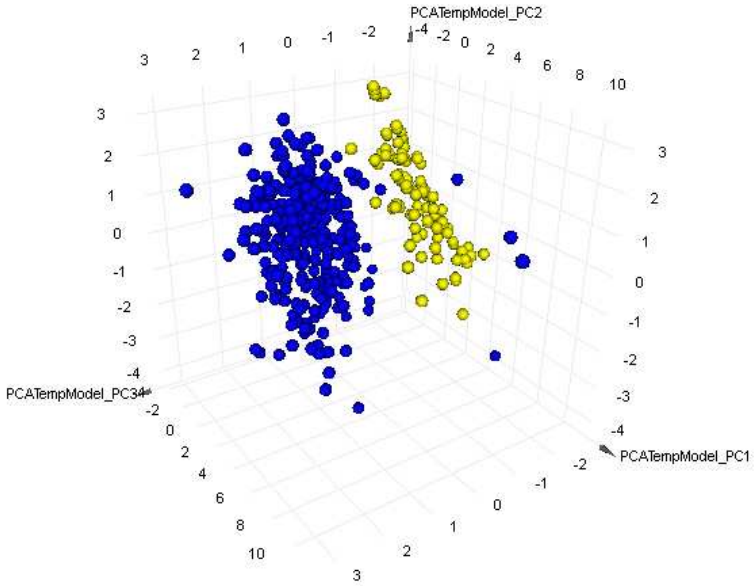
arene-cation

Supplemental Figure 2. Principal component analysis (PCA) of all ToxCast™ compounds (blue spheres) and steroids used in the Bayesian model (yellow spheres) illustrating how the two sets of compounds can be separated in descriptor space (ALogP, molecular weight, number of_hydrogen donors, number of hydrogen bond acceptors, number of rotatable bonds, number of rings, number of aromatic rings, molecular polar surface area and number of atoms). The PCA plot explains 82.1% of total variance in the first 3 principal components. The model was generated with Discovery Studio version 2.1 (Accelrys, San Diego, CA.).